**FIG. 1**

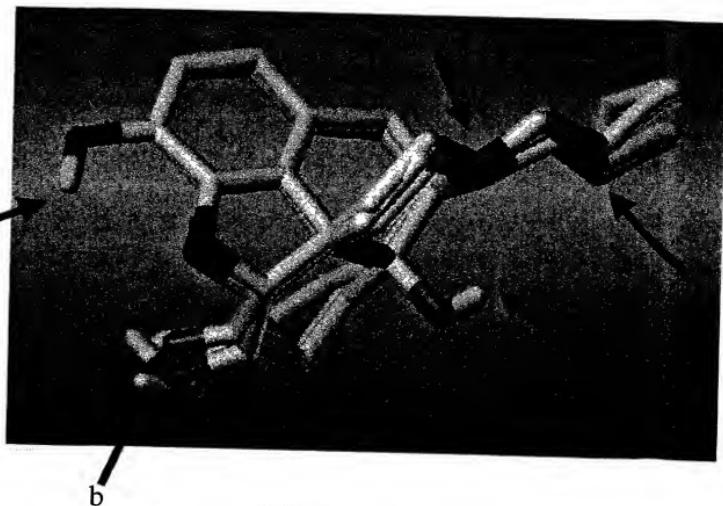


FIG. 2

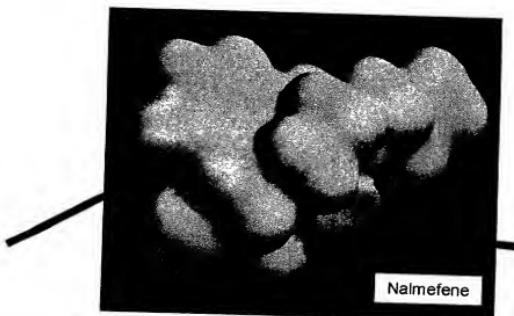


FIG. 3A

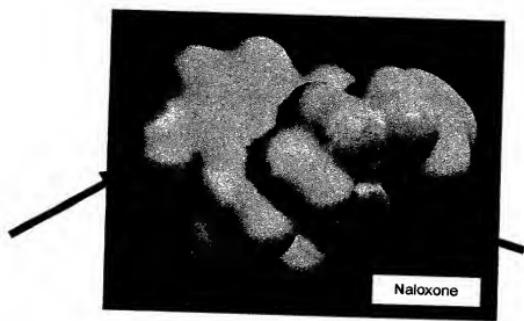


FIG. 3B

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	70413	C ₁₉ H ₂₁ NO ₄	327.384	0.010	Naloxone
	MFCD00133650	C ₂₁ H ₂₅ NO ₃	339.438	0.018	Nalmefene
	349115	C ₂₁ H ₂₇ NO ₃	341.454	0.406	Nalmefene
	BAS 3387173	C ₁₈ H ₂₁ F ₃ N ₂ O ₃	370.375	0.510	Naloxone
	BAS 1002455	C ₁₆ H ₁₉ F ₃ N ₂ O ₃	344.337	0.519	Naloxone
	BAS 3387155	C ₁₇ H ₁₉ F ₃ N ₂ O ₃	356.348	0.524	Naloxone

Fig. 4A

200 Neighbors

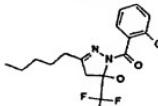
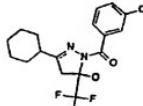
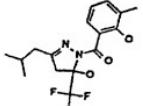
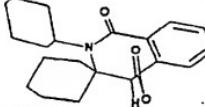
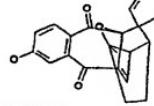
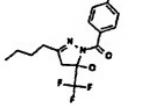
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 1268016	C ₁₆ H ₁₉ F ₃ N ₂ O ₃	344.337	0.534	Naloxone
	BAS 3387156	C ₁₇ H ₁₉ F ₃ N ₂ O ₃	356.348	0.541	Naloxone
	BAS 3387130	C ₁₆ H ₁₉ F ₃ N ₂ O ₃	344.337	0.546	Naloxone
	MFCD01935543	C ₂₁ H ₂₇ NO ₃	341.454	0.551	Naloxone
	688277	C ₂₀ H ₁₈ O ₅	338.363	0.591	S-beta-Nalroxol
	BAS 1002441	C ₁₅ H ₁₇ F ₃ N ₂ O ₃	330.310	0.618	Naloxone

Fig. 4B

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	BAS 3386059	C ₁₆ H ₁₇ F ₃ N ₂ O ₃	342.321	0.637	Naloxone
	BAS 1003176	C ₁₆ H ₁₇ F ₃ N ₂ O ₃	342.321	0.637	Naloxone
	BAS 1004848	C ₁₅ H ₁₇ F ₃ N ₂ O ₃	330.310	0.643	Naloxone
	MFCD00273259	C ₂₁ H ₃₃ NO ₅	379.501	0.644	Nalmefene
	MFCD00273270	C ₂₁ H ₃₁ NO ₅	377.485	0.646	Naloxone
	MFCD00273266	C ₂₁ H ₃₁ NO ₅	377.485	0.648	Naloxone

Fig. 4C

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	BAS 3386023	C ₁₅ H ₁₅ F ₃ N ₂ O ₃	328.294	0.653	Naloxone
	BAS 2026128	C ₁₅ H ₁₅ F ₃ N ₂ O ₃	328.294	0.657	Naloxone
	617005	C ₁₈ H ₂₁ NO ₃	299.373	0.658	6-beta-Naloxone
	MFCDD00079194	C ₁₇ H ₁₉ NO ₄	301.345	0.662	6-beta-Naloxone
	19045	C ₁₇ H ₁₉ NO ₄	301.345	0.666	6-beta-Naloxone
	76021	C ₁₉ H ₂₃ NO ₄	329.399	0.673	Nalmefene

Fig. 4D

200 Neighbors

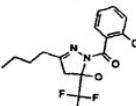
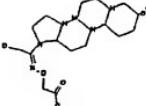
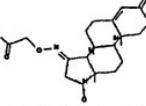
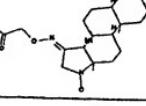
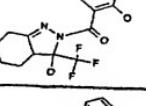
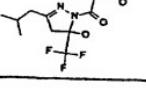
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 1002442	C ₁₅ H ₁₇ F ₃ N ₂ O ₃	330.310	0.677	Naloxone
	MFCD00271723	C ₂₃ H ₃₇ NO ₅	407.555	0.682	Naloxone
	MFCD00273273	C ₂₁ H ₂₉ NO ₅	375.469	0.688	Nalmefene
	MFCD00273264	C ₂₁ H ₃₃ NO ₅	379.501	0.697	Nalmefene
	BAS 2026145	C ₁₆ H ₁₇ F ₃ N ₂ O ₃	342.321	0.698	Naloxone
	BAS 3387114	C ₁₅ H ₁₇ F ₃ N ₂ O ₃	330.310	0.704	Naloxone
.					

Fig. 4E

200 Neighbors

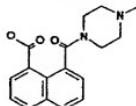
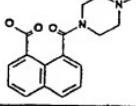
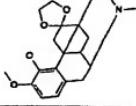
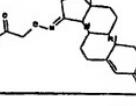
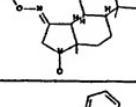
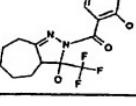
Structure	Cpd ID		MW	Distance	Neighbor
	376679	C ₁₇ H ₁₈ N ₂ O ₃	298.345	0.705	Naloxone
	379963	C ₁₇ H ₁₈ N ₂ O ₃	298.345	0.705	Naloxone
	157670	C ₂₀ H ₂₇ NO ₄	345.442	0.714	Nalmefene
	MFCD00273274	C ₂₁ H ₂₇ NO ₅	373.453	0.720	Naloxone
	MFCD00273260	C ₂₁ H ₃₃ NO ₅	379.501	0.723	Nalmefene
	BAS 1003163	C ₁₆ H ₁₇ F ₃ N ₂ O ₃	342.321	0.727	Naloxone

Fig. 4F

200 Neighbors

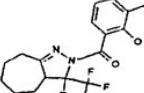
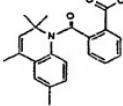
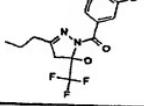
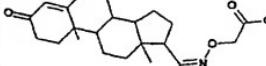
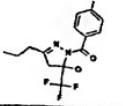
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 1003182	C ₁₇ H ₁₉ F ₃ N ₂ O ₃	356.348	0.739	Naltrexone
	BAS 0510629	C ₂₁ H ₂₁ NO ₃	335.406	0.756	Naltrexone
	BAS 1002419	C ₁₄ H ₁₅ F ₃ N ₂ O ₃	316.282	0.757	Naloxone
	18579	C ₂₃ H ₃₃ NO ₄	387.524	0.760	Nalmefene
	58796	C ₂₃ H ₃₃ NO ₄	387.524	0.760	Nalmefene
	BAS 1004835	C ₁₄ H ₁₅ F ₃ N ₂ O ₃	316.282	0.763	Naloxone

Fig. 4G

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	BAS 2004373	C ₁₇ H ₁₄ F ₃ N ₃ O ₃	365.315	0.765	Naloxone
	693856	C ₁₉ H ₂₄ N ₂ O ₆	376.413	0.768	Nalmefene
	MFCD01764789	C ₁₇ H ₁₇ F ₃ N ₂ O ₃	354.332	0.769	Naloxone
	MFCD00271738	C ₂₃ H ₃₇ NO ₄	391.556	0.772	Nalmefene
	BAS 2025996	C ₁₇ H ₁₄ F ₃ N ₃ O ₃	365.315	0.774	Naloxone
	BAS 2282169	C ₂₂ H ₂₅ NO ₄	367.449	0.780	Nalmefene

Fig. 4H

200 Neighbors

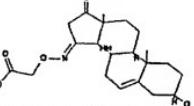
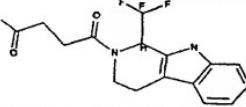
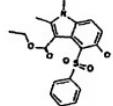
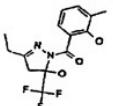
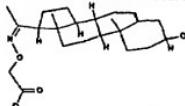
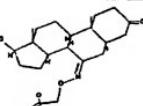
Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00273268	C ₂₁ H ₂₉ NO ₅	375.469	0.789	Naloxone
	MFCD00179880	C ₁₆ H ₁₅ F ₃ N ₂ O ₃	340.305	0.800	Naloxone
	BAS 1507170	C ₁₉ H ₁₉ NO ₅ S	373.431	0.801	Nalmefene
	BAS 3386088	C ₁₄ H ₁₅ F ₃ N ₂ O ₃	316.282	0.802	Naloxone
	MFCD00272052	C ₂₃ H ₃₅ NO ₄	389.540	0.818	Nalmefene
	MFCD00271113	C ₂₁ H ₃₁ NO ₅	377.485	0.829	6-beta-Naltrexol

Fig. 4I

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	116054	C ₁₈ H ₁₉ N ₃ O ₄	341.370	0.831	6-beta-Naltrexol
	BAS 1004837	C ₁₄ H ₁₅ F ₃ N ₂ O ₃	316.282	0.835	Naloxone
	134536	C ₁₉ H ₂₅ NO ₃	315.416	0.836	6-beta-Naltrexol
	615801	C ₁₇ H ₂₀ N ₂ O ₃	300.361	0.856	Naltrexone
	404374	C ₂₀ H ₂₇ NO ₃	329.443	0.870	Nalmefene
	MFCD00273318	C ₂₃ H ₃₅ NO ₄	389.540	0.870	Nalmefene

Fig. 4J

200 Neighbors

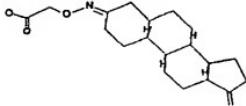
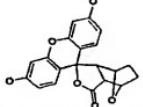
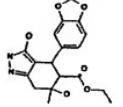
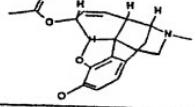
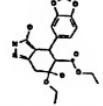
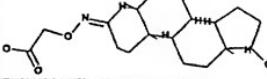
Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00271094		C ₂₁ H ₃₁ NO ₄	361.486	0.877
	202587		C ₂₀ H ₁₆ O ₆	352.347	0.889
	693862		C ₁₈ H ₂₀ N ₂ O ₆	360.370	0.892
	MFCD00467140		C ₁₉ H ₂₁ NO ₄	327.384	0.905
	693863		C ₁₉ H ₂₂ N ₂ O ₇	390.396	0.909
	MFCD00271196		C ₂₁ H ₃₃ NO ₄	363.501	0.912

Fig. 4K

200 Neighbors

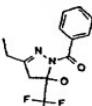
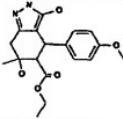
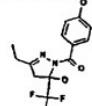
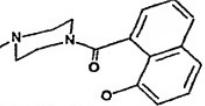
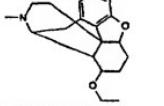
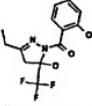
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 3386092	C ₁₃ H ₁₃ F ₃ N ₂ O ₃	302.255	0.919	Naloxone
	693855	C ₁₈ H ₂₂ N ₂ O ₅	346.386	0.923	Nalmefene
	BAS 3386091	C ₁₃ H ₁₃ F ₃ N ₂ O ₃	302.255	0.928	Naloxone
	MFCDO00665833	C ₁₆ H ₁₈ N ₂ O ₂	270.334	0.929	Naltrexone
	404368	C ₁₉ H ₂₅ NO ₃	315.416	0.941	S-beta-Naltrexol
	BAS 0506820	C ₁₃ H ₁₃ F ₃ N ₂ O ₄	318.255	0.948	Naloxone

Fig. 4L

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	693859	C ₁₈ H ₂₂ N ₂ O ₆	362.386	0.949	Nalmefene
	BAS 0436353	C ₁₃ H ₁₃ F ₃ N ₂ O ₃	302.255	0.965	Naloxone
	MFCD00167445	C ₂₀ H ₂₀ N ₂ O ₃	336.394	0.968	Naltrexone
	MFCD00667402	C ₂₁ H ₂₅ NO ₆	387.437	0.974	Nalmefene
	MFCD02258126	C ₁₈ H ₂₅ NO ₆	351.403	0.977	Naloxone
	MFCD00143186	C ₁₉ H ₂₁ NO ₅	343.383	0.985	Naltrexone

Fig. 4M

200 Neighbors

TOOLBOX = 100% SEARCHED

Structure	Cpd ID		MW	Distance	Neighbor
	119887	$C_{21}H_{16}O_5$	348.359	0.993	Naloxone
	404365	$C_{19}H_{25}NO_3$	315.416	1.002	Nalmefene
	MFCD01871411	$C_{21}H_{20}FNO_3$	353.397	1.012	Naloxone
	152720	$C_{18}H_{23}NO_3$	301.389	1.015	δ -beta-Nalroxol
	117581	$C_{22}H_{19}NO_3$	345.402	1.016	Naloxone
	669466	$C_{15}H_{17}N_3O_4$	303.320	1.017	Naloxone

Fig. 4N

200 Neighbors

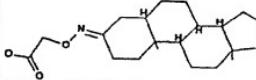
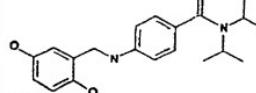
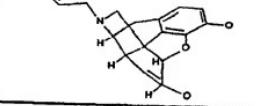
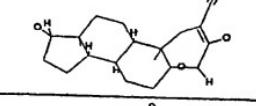
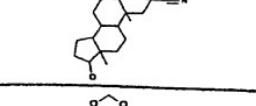
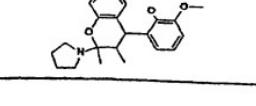
Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00271129	C ₂₁ H ₃₃ NO ₄	363.501	1.029	Nalmefene
	689431	C ₂₀ H ₂₆ N ₂ O ₃	342.442	1.035	6-beta-Naltrexol
	MFCD00056772	C ₁₉ H ₂₁ NO ₃	311.384	1.039	Nalmefene
	MFCD00199295	C ₂₀ H ₂₇ NO ₃	329.443	1.045	Nalmefene
	R191489	C ₂₀ H ₂₇ NO ₃	329.443	1.046	Nalmefene
	375504	C ₂₃ H ₂₇ NO ₅	397.475	1.050	Naloxone

Fig. 4O

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	692397	C ₁₇ H ₁₃ NO ₄	295.297	1.066	Naloxone
	MFCD00433684	C ₁₅ H ₁₅ NO ₃	257.292	1.069	Naloxone
	693860	C ₂₀ H ₂₄ N ₂ O ₆	388.424	1.071	Nalmefene
	MFCD01764791	C ₁₆ H ₁₅ F ₃ N ₂ O ₄	356.304	1.073	Naloxone
	BAS 1519270	C ₂₂ H ₁₉ NO ₃	345.402	1.078	Naloxone
	BAS 3385849	C ₁₂ H ₁₁ F ₃ N ₂ O ₃	288.228	1.083	Naloxone

Fig. 4P

200 Neighbors

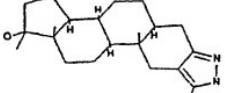
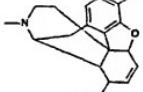
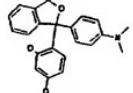
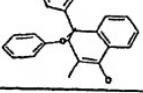
Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00673308	$C_{21}H_{32}N_2O_2$	344.501	1.087	Nalmefene
	404356	$C_{18}H_{21}NO_3$	299.373	1.099	Nalmefene
	43938	$C_{22}H_{19}NO_4$	361.401	1.107	Nalmefene
	117181	$C_{20}H_{20}N_2O_3$	336.394	1.109	Naltrexone
	MFCD00094379	$C_{24}H_{22}O_2$	342.442	1.111	Nalmefene
	404369	$C_{19}H_{25}NO_3$	315.416	1.111	β -beta-Naltrexol

Fig. 4Q

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	381577	$C_{21}H_{25}NO_7$	403.436	1.111	Naloxone
	S842214	$C_{24}H_{22}O_2$	342.442	1.112	Nalmefene
	134602	$C_{19}H_{21}NO_4$	327.384	1.112	6-beta-Naltrexol
	CHS 0316796	$C_{18}H_{25}N_3O_3$	331.418	1.113	Naloxone
	134604	$C_{20}H_{25}NO_4S$	375.491	1.115	Nalmefene
	R171697	$C_{23}H_{27}NO_5$	397.475	1.133	Nalmefene

Fig. 4R

200 Neighbors

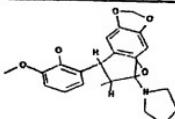
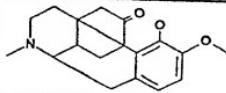
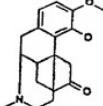
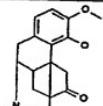
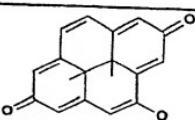
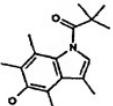
Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00667401	$C_{23}H_{27}NO_5$	397.475	1.134	Nalmefene
	S959863	$C_{18}H_{24}ClNO_3$	337.850	1.137	6-beta-Naloxone
	35545	$C_{18}H_{23}NO_3$	301.389	1.137	6-alpha-Naloxone
	134598	$C_{18}H_{23}NO_3$	301.389	1.137	6-gamma-Naloxone
	S310778	$C_{18}H_{14}O_3$	278.310	1.140	Naloxone
	669800	$C_{17}H_{23}NO_2$	273.378	1.141	Naloxone

Fig. 4S

200 Neighbors

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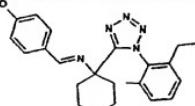
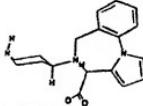
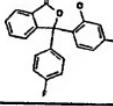
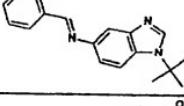
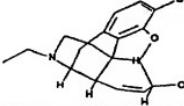
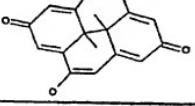
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 0083962	C ₂₃ H ₂₇ N ₅ O	389.505	1.141	Naltrexone
	MFCD01765597	C ₁₈ H ₂₁ N ₃ O ₂	311.387	1.142	6-beta-Naltrexol
	682334	C ₂₁ H ₁₅ FO ₃	334.350	1.143	Naloxone
	BAS 0631739	C ₁₈ H ₁₉ N ₃ O	293.372	1.143	Nalmefene
	MFCD00144882	C ₁₈ H ₂₁ NO ₃	299.373	1.149	6-beta-Naltrexol
	MFCD00229975	C ₁₈ H ₁₄ O ₃	278.310	1.150	Naloxone

Fig. 4T

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	R171700	$C_{21}H_{25}NO_6$	387.437	1.157	Nalmefene
	134592	$C_{19}H_{23}NO_3$	313.400	1.163	β -beta-Naltrixol
	401210	$C_{23}H_{18}O_2$	326.399	1.166	Nalmefene
	BAS 2026074	$C_{17}H_{17}N_3O_3$	311.343	1.172	Naltrexone
	BAS 3050727	$C_{21}H_{25}F_3N_2O_3$	410.440	1.177	Nalmefene
	BAS 0341630	$C_{12}H_{11}F_3N_2O_3$	288.228	1.185	Naloxone

Fig. 4U

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	97817	C ₁₈ H ₂₃ NO ₄	317.388	1.190	Naloxone
	ASN 3185453	C ₂₄ H ₂₈ O ₄	380.488	1.196	Naloxone
	21257	C ₁₈ H ₁₉ NO ₃	297.357	1.196	6-beta-Naltrexol
	134601	C ₁₈ H ₂₁ NO ₃	299.373	1.200	6-beta-Naltrexol
	BAS 2026075	C ₁₇ H ₁₇ N ₃ O ₃	311.343	1.203	6-beta-Naltrexol
	BAS 1996620	C ₁₈ H ₁₅ N ₃ O ₃	297.316	1.211	6-beta-Naltrexol

Fig. 4V

200 Neighbors

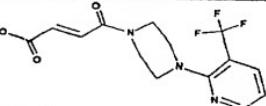
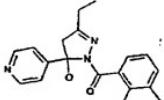
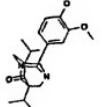
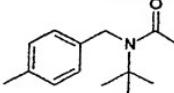
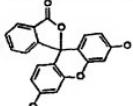
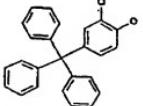
Structure	Cpd ID		MW	Distance	Neighbor
	MFCD01314356	$C_{14}H_{14}F_3N_3O_3$	329.281	1.215	Naloxone
	BAS 2026097	$C_{18}H_{19}N_3O_3$	325.370	1.221	Naltrexone
	BAS 1914007	$C_{21}H_{30}N_2O_3$	358.485	1.221	Naloxone
	CHS 0003221	$C_{16}H_{21}NO_3$	275.351	1.227	Naloxone
	667258	$C_{20}H_{12}O_5$	332.316	1.227	Naloxone
	37625	$C_{25}H_{20}O_2$	352.437	1.235	Nalmefene

Fig. 4W

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	BAS 1003093	C ₁₆ H ₁₅ N ₃ O ₃	297.316	1.236	6-beta-Nalrox
	16468	C ₂₀ H ₁₄ O ₄	318.332	1.238	Naloxone
	CHS 0227049	C ₁₈ H ₂₃ NO ₃	301.389	1.241	Naloxone
	BAS 0315050	C ₂₂ H ₂₄ N ₄ O ₂	376.462	1.241	Nalmefene
	BAS 1289763	C ₁₈ H ₂₃ NO ₃	301.389	1.242	Naloxone
	349127	C ₁₇ H ₁₉ NO ₄	301.345	1.243	Naloxone

Fig. 4X

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	635928	C ₁₈ H ₂₀ O ₆	332.356	1.250	Nalmefene
	BAS 2377555	C ₁₇ H ₁₇ N ₃ O ₃	311.343	1.251	6-beta-Naltraxol
	MFCD00665835	C ₁₅ H ₁₅ NO ₂	241.292	1.251	Naltrexone
	47931	C ₁₉ H ₂₃ NO ₂	297.401	1.255	6-beta-Naltraxol
	76435	C ₁₈ H ₂₁ NO ₃	299.373	1.257	Nalmefene
	90558	C ₂₁ H ₂₆ NO ₄	356.446	1.258	Naloxone

Fig. 4Y

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00206273	$C_{20}H_{21}N_3O_2$	335.409	1.261	Naloxone
	159208	$C_{17}H_{19}NO_4$	301.345	1.267	Nalmefene
	BAS 0341580	$C_{16}H_{13}ClN_2O_3$	316.747	1.267	Naltrexone
	BAS 2377575	$C_{18}H_{19}N_3O_3$	325.370	1.268	Naltrexone
	MFCD01765638	$C_{19}H_{17}N_3O_2$	319.366	1.268	Nalmefene
	R171484	$C_{20}H_{23}NO_5$	357.410	1.268	Nalmefene

Fig. 4Z

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	700350	$C_{15}H_{23}N_5O_2$	305.383	1.272	Naloxone
	16907	$C_{20}H_{15}NO_4$	333.347	1.274	Nalmefene
	R170623	$C_{21}H_{25}NO_5$	371.437	1.275	Nalmefene
	S88907	$C_{20}H_{14}O_4$	318.332	1.278	Naloxone
	10464	$C_{20}H_{14}O_4$	318.332	1.278	Naloxone
	215214	$C_{20}H_{14}O_4$	318.332	1.278	Naloxone

Fig. 4AA

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	R171425	C ₂₀ H ₂₃ NO ₅	357.410	1.280	Nalmefene
	MFCD00153032	C ₁₇ H ₁₉ NO ₃	285.346	1.283	6-beta-Naltri xol
	S196991	C ₁₉ H ₁₉ NO ₃	309.368	1.285	Naltrexone
	R170291	C ₂₀ H ₂₃ NO ₆	373.409	1.286	Naloxone
	682335	C ₂₁ H ₁₅ FO ₃	334.350	1.287	Naloxone
	MFCD00567377	C ₂₀ H ₂₃ NO ₅	357.410	1.289	Nalmefene

Fig. 4AB

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	106242	C ₂₁ H ₂₀ N ₂ O ₂	332.408	1.294	Naloxone
	R170410	C ₂₀ H ₂₃ NO ₆	373.409	1.299	Naloxone
	MFCD00005912	C ₂₂ H ₁₈ O ₄	346.386	1.300	Naloxone
	MFCD01765637	C ₂₀ H ₁₈ N ₂ O ₂	318.379	1.302	Nalmefene
	376678	C ₁₇ H ₂₀ N ₂ O ₃	300.361	1.303	Neltrexone
	MFCD01314431	C ₁₈ H ₁₆ F ₃ N ₃ O ₃	379.342	1.303	Naloxone

Fig. 4AC

200 Neighbors

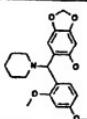
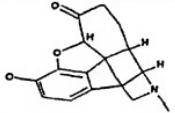
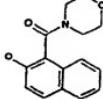
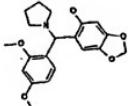
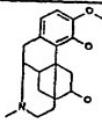
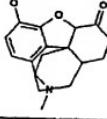
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	370278	$C_{21}H_{25}NO_5$	371.437	1.304	Nalmefene
	MFCD00242635	$C_{17}H_{19}NO_3$	285.346	1.305	6-beta-Naloxane
	S602965	$C_{15}H_{15}NO_3$	257.292	1.306	Nalrexone
	370279	$C_{20}H_{23}NO_5$	357.410	1.306	Nalmefene
	157877	$C_{18}H_{25}NO_3$	303.405	1.310	Nalmefene
	19046	$C_{17}H_{19}NO_3$	285.346	1.310	6-beta-Naloxane

Fig. 4AD

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	117862	C ₁₇ H ₁₉ NO ₃	285.346	1.310	6-beta-Naltrexol
	MFCD00667305	C ₂₁ H ₂₅ NO ₅	371.437	1.313	Nalmefene
	MFCD00667382	C ₂₀ H ₂₃ NO ₅	357.410	1.316	Nalmefene
	611276	C ₁₇ H ₁₉ NO ₃	285.346	1.318	6-beta-Naltrexol
	BAS 1099232	C ₂₁ H ₂₂ N ₂ O ₃	350.421	1.320	Naltrexone
	BAS 0313319	C ₁₈ H ₁₈ N ₂ O ₃	310.356	1.321	6-beta-Naltrexol

Fig. 4AE

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	401211	C ₂₃ H ₁₈ O ₃	342.398	1.325	Nalmefene
	409635	C ₁₈ H ₁₇ NO ₂	279.342	1.326	Nalmefene
	106231	C ₂₃ H ₂₄ N ₂ O ₂	360.460	1.327	Naloxone
	375505	C ₂₂ H ₂₅ NO ₅	383.448	1.329	Naloxone
	BAS 1053035	C ₂₀ H ₁₅ NO ₃	317.347	1.331	Naloxone
	ASN 3160807	C ₂₂ H ₂₄ O ₄	352.434	1.332	Naloxone

Fig. 4AF

200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	324633	$C_{21}H_{26}O_6$	374.438	1.333	Naloxone
	370277	$C_{20}H_{23}NO_6$	373.409	1.339	Naloxone
	MFCD00375811	$C_{20}H_{15}NO_4$	333.347	1.343	6-beta-Naltrexol
	BAS 0659522	$C_{20}H_{15}NO_4$	333.347	1.343	6-beta-Naltrexol
	CHS 0305736	$C_{20}H_{15}NO_4$	333.347	1.343	6-beta-Naltrexol
	381576	$C_{20}H_{23}NO_6$	373.409	1.348	Naloxone

Fig. 4AG

200 Neighbors

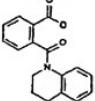
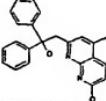
Structure	Cpd ID		MW	Distance	Neighbor
	CHS 0120289	C ₁₇ H ₁₅ NO ₃	281.314	1.348	Naloxone
	351159	C ₂₃ H ₂₀ N ₂ O ₂	356.426	1.349	Nalmefene

Fig. 4AH